ABSTRACT OF THE DISCLOSURE

There is provided a molecular reaction characteristic predicting method capable of accurately predicting the presence of similarity between reaction characteristic of various molecules without limitations on common molecular skeleton.

A molecule surrounding surface (20) is set so as to be reflected in the spatial dimension of a molecule, and a molecule surrounding space surrounded by the molecule surrounding surface is divided into a plurality of component spaces (22), by which the reaction characteristic of the molecule is characterized. Then, probe points are provided on a frontier surrounding surface (5) on the molecule surrounding surface, and a space occupied rate is derived for each of the component spaces. Then, electrostatic energies are derived for each of the probe points on the frontier surrounding surface, and the sum of the electrostatic energies on the frontier surrounding surface is derived as an electrostatic factor of each of the component spaces. In addition, van der Waals energies are derived for each of the probe points, and the sum of the van der Waals energies on the frontier surrounding surface is derived as a steric factor of each of the component spaces. Then, assuming that the space occupied rate, the electrostatic factor and the steric factor are reaction characteristic values of the corresponding one of the component spaces, the reaction characteristic of the molecule is predicted on the basis of the reaction characteristic values of each of the component spaces.